Effective on 12/08/2004.
Fees pursuant to the Consolidated Appropriations Act, 2005 (H.R. 4818).

FEE TRANSMITTAL for FY 2006

☐ applicant claims small entity status. See 37 CFR 1.27.

TOTAL AMOUNT OF PAYMENT	($) 500.00

Complete if Known	
Application Number	09/506,741
Filing Date	February 18, 2000
First Named Inventor	Victor S. Lobanov
Examiner Name	Lori A. Clow
Art Unit	1631
Attorney Docket No.	30923-715.201

METHOD OF PAYMENT (check all that apply)

☐ Check ☐ Credit card ☐ Money Order ☐ None ☐ Other (please identify): _____

☒ Deposit Account: Deposit Account Number: 23-2415 Deposit Account Name: Wilson Sonsini Goodrich & Rosati

For the above-identified deposit account, the Director is hereby authorized to: (check all that apply)

☒ Charge fee(s) indicated below ☐ Charge fee(s) indicated below, **except for the filing fee**

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FEE CALCULATION

1. BASIC FILING, SEARCH, AND EXAMINATION FEES

	FILING FEES		SEARCH FEES		EXAMINATION FEES		
		Small Entity		Small Entity		Small Entity	
Application Type	Fee ($)	Fee ($)	Fee ($)	Fee ($)	Fee ($)	Fee ($)	Fees Paid ($)
Utility	300	150	500	250	200	100	
Design	200	100	100	50	130	65	
Plant	200	100	300	150	160	80	
Reissue	300	150	500	250	600	300	
Provisional	200	100	0	0	0	0	

2. EXCESS CLAIM FEES

Fee Description	Fee ($)	Small Entity Fee ($)
Each claim over 20 or, for Reissues, each claim over 20 and more than the original patent	50	25
Each independent claim over 3 or, for Reissues, each independent claim more than in the original patent	200	100
Multiple dependent claims	360	180

Total Claims		Extra Claims	Fee ($)		Fee Paid ($)
_____	- 20 or HP =	_____	x _____	=	_____

HP = highest number of total claims paid for, if greater than 20

Indep. Claims		Extra Claims	Fee ($)		Fee Paid ($)
_____	- 3 or HP =	_____	x _____	=	_____

HP = highest number of total claims paid for, if greater than 3

Multiple Dependent Claims	
Fee ($)	Fee Paid ($)
_____	_____

3. APPLICATION SIZE FEE

If the specification and drawings exceed 100 sheets of paper (excluding electronically filed sequence or computer listings under 37 CFR 1.52(e)), the application size fee due is $250 ($125 for small entity) for each additional 50 sheets or fractions thereof. See 35 U.S.C. 41(a)(1)(G) and 37 CFR 1.16(s).

Total Sheets		Extra Sheets		Number of each additional 50 or fraction thereof		Fee ($)		Fee Paid ($)
_____	- 100 =	_____	/ 50 =	_____	(round **up** to a whole number)	x _____	=	_____

4. OTHER FEE(S)

	Fees Paid ($)
Non-English Specification, $130 fee (no small entity discount)	
Other: Filing brief in support of appeal	**$500.00**

SUBMITTED BY

Signature	Samir Elamrani	Registration No. (Attorney/Agent) 43,601	Telephone 650-493-9300
Name (Print/Type)	Samir Elamrani, Ph.D.		Date March 14, 2006

This collection of information is required by 37 CFR 1.136. The information is required to obtain or retain a benefit by the public which is to file (and by the USPTO to process) an application. Confidentiality is governed by 35 U.S.C. 122 and 37 CFR 1.14. This collection is estimated to take 30 minutes to complete, including gathering, preparing, and submitting the completed application form to the USPTO. Time will vary depending upon the individual case. Any comments on the amount of time you require to complete this form and/or suggestions for reducing this burden, should be sent to the Chief Information Officer, U.S. Patent and Trademark Office, U.S. Department of Commerce, P.O. Box 1450, Alexandria, VA 22313-1450. DO NOT SEND FEES OR COMPLETED FORMS TO THIS ADDRESS. **SEND TO: Commissioner for Patents, P.O. Box 1450, Alexandria, VA 22313-1450.**

If you need assistance in completing the form, call 1-800-PTO-9199 and select option 2.

WSGR Reference No. 30923-715.201

IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

In re the Patent Application of: Applicants: Lobanov *et al.* Serial No.: 09/506,741 Filed: February 18, 2000 Title: *System, Method and Computer Program Product For Fast and Efficient Searching of Large Chemical Libraries*	Group Art Unit: 1631 Examiner: Lori A. Clow WSGR Reference No.: 30923-715.201 Certificate of Mailing Under C.F.R. §1.8 I hereby certify that this correspondence and all marked attachments are being deposited by Express Mail, Express Mailing Label No.: EV 334638387 on March 14, 2006, addressed to: Mail Stop Appeal Brief -- Patents, Commissioner for Patents, P.O. Box 1450, Alexandria, VA 22313-1450. By: Vicki L. Andrews Vicki L. Andrews

APPEAL BRIEF UNDER 37 C.F.R. § 41.37

MAIL STOP APPEAL BRIEF - PATENTS
Commissioner for Patents
P.O. Box 1450
Alexandria, VA 22313-1450

Sir:

Applicants hereby appeal from the Final Rejection of June 15, 2005. This is being filed along with a one month Petition for Extension of Time and within three-months of filing the Notice of Appeal, filed on December 14, 2005.

The fees required under § 1.17, and any required petition for extension of time for filing this brief and fees thereof, are dealt with in the accompanying TRANSMITTAL OF APPEAL BRIEF.

REAL PARTY IN INTEREST

The assignee identified in the assignment recorded in the USPTO on February 18, 2000, at Reel/Frame 010631/0565, 3-Dimensional Pharmaceuticals, Inc., has merged into Johnson & Johnson Pharmaceutical Research & Development, L.L.C. Thus, the real party of interest is Johnson & Johnson Pharmaceutical Research & Development, L.L.C., which is a subsidiary of Johnson & Johnson.

RELATED APPEALS AND INTERFERENCES

There are no other prior or pending appeals, judicial proceedings, or interferences known to Appellants, the undersigned legal representative of Appellants, or the above-identified assignee that would directly affect, be directly affected by, or having a bearing on the Board's decision in the present appeal, as reflected in the Related Proceedings Appendix.

STATUS OF CLAIMS

Claims 1, 2, 7, 8, 10-26, 31, 32 and 34-48 are currently pending in the application at the time of the filing of the Notice of Appeal. Claims 3-6, 9, 27-30 and 33 had been cancelled previously. A true copy of the claims on appeal is presented in the Appendix. No claims have been allowed.

STATUS OF AMENDMENTS

The amendments submitted March 9, 2005 have been entered and appear in the claims on appeal. No amendments have been submitted subsequent to the final Office Action.

SUMMARY OF CLAIMED SUBJECT MATTER

The claimed invention relates to screening enumerated or non-enumerated virtual libraries using a computer-implemented method of analyzing the libraries. The claimed invention also relates to computer based systems and computer program products capable of performing the analysis.

Claims 1, 13, 20, 23 and 24 are independent claims directed to various aspects of a computer implemented method of analyzing a non-enumerated virtual library, a computer based system for analyzing a non-enumerated virtual library, and computer program product comprising a computer useable medium having computer program logic recorded thereon for enabling a processor to analyze a non-enumerated virtual library. . By way of example, claim 1 on appeal is directed to a computer implemented method of analyzing a non-enumerated virtual library, comprising:

(a) randomly selecting a set of N reagent combinations from the non-enumerated virtual library, wherein said selected N reagent combinations represent a set of N compounds;

(b) enumerating said set of N compounds;

(c) selecting M compounds from said set of N enumerated compounds wherein the selection of M compounds from said set of N enumerated compounds is based on at least one fitness function;

(d) deconvoluting said M compounds into their associated building blocks;

(e) generating said focused library of at least one compound based on said building blocks; and

(f) enumerating at least one compound in said focused library of at least one compound;

(g) selecting at least one K compound; and

(h) synthesizing said at least one K compound.

Support for independent claims 1, 13, 20, 23 and 24 can be found in the specification as filed, such as, for example, at page 8, line 2 through page 9, line 7; at page 17, line 16 through page 21, line 5; page 47, lines 23-24; page 47, lines 18-22; and in Figures 1, 5, 6, 7 and 8.

Claims 25, 47 and 48 are independent claims directed to a computer implemented method of analyzing an enumerated virtual library, to a computer based system for analyzing an enumerated virtual library, and a computer program product comprising a computer useable medium having computer program logic recorded thereon for enabling a processor to analyze an enumerated virtual library. Support for independent claims 25, 47 and 48 can be found in the specification as filed, such as, for example, at page 8, lines 2-15; at page 9, lines 23-27; at page 21, line 6 through page 23, line 10; page 47, lines 18-22; and in Figure 1A. Support for computer program product, computer based systems, computer program medium and computer usable medium can be found in the specification as filed, such as, for example, at page 47, lines 1-10; at page 50, line 1 through page 51, line 12; and in Figures 19 and 20.

Additionally, support for the following means-plus-function language as recited in independent claims 23 and 47 can be found in the specification as noted below:

i. means for randomly selecting a set of N reagent combinations from the virtual library, wherein said selected N reagent combinations represent a set of N compounds: a property prediction algorithm or a quantitative structure-activity model, a biomolecular docking algorithm, 2D or 3D QSAR predictions, and receptor complementarity (page 15, line 10 through page 17, line 15; page 21, lines 14-25);

ii. means for enumerating said set of N compounds: page 47, lines 1-10; page 51, line 13 through page 52, line 4, and Figures 19 and 20;

iii. means for selecting M compounds of said set of N enumerated compounds based on a fitness function: a stochastic version of a maximin algorithm, Monte-Carlo sampling protocol, a Simulated Annealing protocol or variants thereof, DirectedDiversity® API toolkit (page 30, line 26 through page 32, line 24; and page 38, lines 7-27);

iv. means for deconvoluting said M compounds into their associated building blocks: page 47, lines 1-10, pages 50-52 and in Figures 19 and 20;

v. means for generating said focused library of compounds based on said building blocks: page 47, lines 1-10, pages 50-52 and in Figures 19 and 20;

vi. means for enumerating a plurality of said compounds of said focused library of compounds: page 47, lines 1-10, pages 50-52 and in Figures 19 and 20; and

vii. means for selecting at least one K compound of said enumerated compounds of said focused library based on the fitness function: a selection algorithm, Monte-Carlo sampling protocol, a Simulated Annealing protocol or variants thereof (page 33, lines 1-21; page 34, lines 25-28; and page 36, lines 8-10).

Moreover, support for the following means-plus-function language as recited in independent claims 24 and 48 is noted below:

i. a first function that enables the processor to randomly select a set of N enumerated compounds from the enumerated virtual library: a property prediction algorithm or a quantitative structure-activity model, a biomolecular docking algorithm, 2D or 3D QSAR predictions, and receptor complementarity (page 15, line 10 through page 17, line 15; page 21, lines 14-25);

ii. a second function that enables the processor to select M compounds of said set of N enumerated compounds based on the fitness function: a stochastic version of a maximin algorithm, Monte-Carlo sampling protocol, a Simulated Annealing protocol or variants thereof, DirectedDiversity® API toolkit (page 30, line 26 through page 32, line 24; and page 38, lines 7-27);

iii. a third function that enables the processor to deconvolute said M compounds into associated building blocks: page 47, lines 1-10, pages 50-52 and in Figures 19 and 20;

iv. means for extracting an enumerated focused library, based on said associated building blocks from the enumerated virtual library, wherein said enumerated focused library includes S enumerated compounds: page 47, lines 1-10, pages 50-52 and in Figures 19 and 20;

v. a fourth function that enables the processor to select at least one K compound of said S enumerated compounds based on the fitness function: a selection algorithm, Monte-Carlo sampling protocol, a Simulated Annealing protocol or variants thereof (page 33, lines 1-21; page 34, lines 25-28; and page 36, lines 8-10); and

vi. a fifth function that enables the processor to select at least one K compound from said S enumerated compounds, wherein K < S, wherein at least one selected K compound is synthesized: a selection algorithm, Monte-Carlo sampling protocol, a Simulated Annealing protocol or variants thereof (page 33, lines 1-21; page 34, lines 25-28; and page 36, lines 8-10).

GROUNDS OF REJECTION TO BE REVIEWED ON APPEAL

Whether claims 1, 2, 7, 8, 10-26, 31, 32 and 34-48 are patentable under 35 U.S.C. § 102(e) over Cramer *et al.* (U.S. Patent No. 6,240,374 B1).

GROUPING OF CLAIMS

Solely for purposes of the present appeal, the patentability of claims 1, 2, 7, 8, 10-26, 31, 32 and 34-48 may be treated as standing or falling together.

ARGUMENTS

Contrary to the position of the Examiner, claims 1, 2, 7, 8, 10-26, 31, 32 and 34-48 are not anticipated under 35 U.S.C. § 102(e) by Cramer. In the Office Action dated December 9, 2004, claims 1-3, 7-27 and 31-48 were rejected under 35 U.S.C. § 102(e) as being anticipated by Cramer. The Examiner indicated that Cramer is "directed to a virtual library creation and searching for [a] molecule with characteristics similar to a selected molecule." With respect to claims 1, 23-25, 47, and 48, the Examiner indicated that Cramer describes: "a non-enumerated virtual library generated

from structural variations of any one synthetic reaction," "from this library a random selection is generated," "this selection is enumeration as a 0.001 fraction," "a fitness function in the form of bits evaluated in the Tanimoto fingerprint," "a subset of compounds is selected with certain Tanimoto similarities of 0.80 or higher or, alternatively other such criteria values," and a "structural core, and other structural building blocks defined as the core, fpcard and fp," "[s]imilarity searches to produce a screening or focused library," and the "number of focused or screening library fingerprint structural variations that are searched are enumerated." Regarding claims 2 and 26, the Examiner further indicated that Cramer discusses "[a]n output of the results." With respect to claims 3 and 27, the Examiner indicated that Cramer discusses "the selection of compounds." And regarding claims 7-9, the Examiner indicated that Cramer discusses the "output[ting] of results defined via similarity evaluation." This position was maintained in the final rejection set forth in the Office Action dated June 15, 2006. In the Advisory Action mailed December 16, 2005, the Examiner supplemented the final rejection by citing column 66, lines 45-55 and column 67, lines 9-11 of Cramer as teaching steps (d) [deconvoluting said M compounds into their associated building blocks] and (e) [generating said focused library of at least one compound based on said building blocks] of the independent claims. The Examiner indicated that the structural variation files and cores as disclosed by the indicated columns and lines were being interpreted as "building blocks" of files. The Examiner stated that "[t]his is equivalent to a deconvolution step, or a breaking down into elements. Further column 68, lines 15-26 teach the virtual generation of a 'focused' library."

The Examiner's rejection, however, is in error since Cramer does not disclose each and every element of the claimed methods, systems and products. As noted by the Federal Circuit, anticipation under 35 U.S.C. § 102 occurs only "when the same device or method, having all of the elements contained in the claim limitations, is described in a single prior art reference." Crown Operations International, Ltd. v. Solutia, Inc., 289 F.3d 1367 (Fed. Cir. 2002). "A single prior art reference anticipates a patent claim if it expressly or inherently describes each and every limitation set forth in the patent claim." Trintec Industries, Inc. v. Top-U.S.A. Corp., 295 F.3d 1292 (Fed. Cir. 2002). Moreover, the "single reference must describe the claimed invention with sufficient precision and

detail to establish that the subject matter existed in the prior art." Verve, LLC v. Crane Cams, Inc., 311 F.3d 1116 (Fed. Cir. 2002)

Cramer discloses a method based on using validated descriptors to generate a virtual library of potential product molecules. The library may be formed by combinatorial arrangement of structural variations and cores. The validated descriptors can be used to select and create optimal diverse subsets, from which subsets, molecules with characteristics similar to a selected molecule can be identified. The virtual library described by Cramer creates the library based on Topomeric CoMFA Descriptors and Tanimoto Fingerprint Descriptors. The library is then filtered by the removal of reactants for non-diversity reasons, removal of non-diversity reactants, removal of products for non-diversity reasons, and removal of non-diversity products. The next step involves merging libraries, and searching the virtual library. See Cramer at col. 13-77. According to the disclosure in Cramer, as the fingerprint metric of the virtual library is calculated for each set of structural variations attached to a specific core, separate structural variations files containing the fingerprint data are required for each combination of core with the structural variations. See Cramer at lines 42-52 of column 66. Then, rather than using the library described above, a new library is constructed by locating the fingerprinting files associated with each structural variation file and different cores in separate files. See Cramer at lines 52-55 of column 66. This new library can be used with more than one cSLN as long as the same type of chemical reaction is used. See Cramer at lines 65-67 of column 66. Furthermore, Cramer, at column 66, lines 45-55, teaches the following: "[w]hen initially constructed the virtual library consisted of the files described above. However, since the fingerprint metric is calculated for each set of structural variations attached to a specific core, separate structural variations files containing the fingerprint data were required for each combination of core with the structural variations. The virtual library therefore contained a great deal of redundant data (structural variation files repetitively containing the same non-fingerprint data). Accordingly, a more efficient virtual library is constructed by locating the fingerprint files associated with each structural variation file and different cores in separate file."

In contrast with the presently claimed invention, Cramer does not disclose or suggest deconvoluting M compounds into their associated building blocks and generating a focused library

of at least one compound based on the building blocks in the context of the other elements recited in each of the independent claims. Cramer only discusses a virtual library created based on Topomeric CoMFA Descriptors and Tanimoto Fingerprint Descriptors, which is purportedly filtered by the removal of reactants for non-diversity reasons, removal of non-diversity reactants, removal of products for non-diversity reasons, and removal of non-diversity products. The next step involves merging libraries, and searching the virtual library. Cramer does not describe deconvoluting M compounds into their associated building blocks and generating a focused library of at least one compound based on the building blocks.

Neither the section relied upon in the Office Action, nor any other section of Cramer discloses the step of generating smaller focused library of at least one compound based on building blocks selected as preferred reagents. See, e.g., page 19, lines 12-19, of the present specification (emphasis added):

[o]nce M compounds are selected, based on the fitness function, from the first set of enumerated compounds, these M compounds are deconvoluted into their building blocks (i.e. reagents), in step 110.

In step 112, the building blocks resulting from step 110 are combined into lists of "preferred" reagents and are used to produce a smaller "focused" library. This focused library can be thought of as a sub-matrix of the larger matrix that represents the entire original virtual combinatorial library.

Apparently, the Examiner has misconstrued the teachings of Cramer at lines 45-55 of column 66, because the paragraph cited by the Examiner describes construction of two (2) distinct virtual libraries. The first library is discussed in Cramer at column 66, lines 45-52 (emphasis supplied): "[w]hen initially constructed the virtual library consisted of the files described above. However, since the fingerprint metric is calculated for each set of structural variations attached to a specific core, separate structural variations files containing the fingerprint data were required for each combination of core with the structural variations. The virtual library therefore contained a great deal of redundant data (structural variation files repetitively containing the same non-fingerprint

data)." The second library is discussed in Cramer at lines 52-55 of column 66 (emphasis added): "[a]ccordingly, a more efficient virtual library is constructed by locating the fingerprint files associated with each structural variation file and different cores in separate files." Cramer further teaches at lines 65-67 of column 66 (emphasis supplied) that the same structural variation files of this second library "may now be used with more than one cSLN as long as the same type of chemical reaction is involved."

This second library is not a further embodiment of the first library. Rather, it is construction of an alternative library embodiment in which fingerprint files are associated with each structural variation file and different cores in separate files. Thus, this section of Cramer describes the method in which files were established during the construction of a separate library based on structural variations and combinations of core. Further, the feature that the second library of Cramer can be used with more than one cSLN as long as the same type of chemical reaction is involved is not the same as the feature of the claimed invention providing for random searching of a library followed by a selection of M compounds which are deconvoluted into their building blocks (i.e., reagents) and used to generate a more focused library.

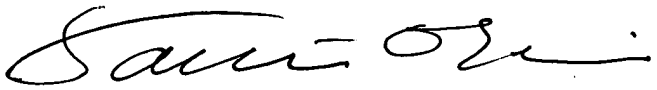
One of ordinary skill in the art would not have interpreted that Cramer's construction of a new library for search purposes constitutes or suggests deconvoluting a selected group of M compounds (generated from a random search) into their associated building blocks (i.e., reagents) and generating the focused library of at least one compounds based on said building blocks, as recited in steps (d) and (e) of each independent claim of the present application. Thus, the independent claims as well as the claims dependent thereon patentably define over Cramer.

CONCLUSION

Applicants believe that for the reasons set forth above, the rejection of claims 1, 2, 7, 8, 10-26, 31, 32 and 34-48 under 35 U.S.C. § 102(e)(2) based on Cramer is in error and should be reversed.

Respectfully submitted,

WILSON SONSINI GOODRICH & ROSATI
Professional Corporation



Date: March 14, 2006

Samir Elamrani, Attorney for Applicants
Registration No. 43,601

CLAIMS APPENDIX

1. (Previously Presented) A computer implemented method of analyzing a non-enumerated virtual library, comprising:

(a) randomly selecting a set of N reagent combinations from the non-enumerated virtual library, wherein said selected N reagent combinations represent a set of N compounds;

(b) enumerating said set of N compounds;

(c) selecting M compounds from said set of N enumerated compounds wherein the selection of M compounds from said set of N enumerated compounds is based on at least one fitness function;

(d) deconvoluting said M compounds into their associated building blocks;

(e) generating said focused library of at least one compound based on said building blocks; and

(f) enumerating at least one compound in said focused library of at least one compound;

(g) selecting at least one K compound; and

(h) synthesizing said at least one K compound.

2. (Previously Presented) The method of claim 1, wherein said focused library of at least one compound includes a plurality of compounds, further comprising:

(i) selecting at least one K compound from said focused library of compounds, and outputting a list of said at least one K compound.

7. (Previously Presented) The method of claim 1, wherein the at least one fitness function in step (c) is selected from similarity, diversity, and presence or absence at least one characteristic.

8. (Previously Presented) The method of claim 7, wherein said focused library of at least one compound includes a plurality of compounds, wherein step (g) further comprises: selecting at least one K compound from said focused library of compounds based on said fitness function and outputting a list of said at least one K compound.

10. (Previously Presented) The method of claim 8, wherein step (c) comprises:

(i) selecting an initial sub-set of M compounds from said set of N enumerated compounds;

(ii) evaluating said initial sub-set of M compounds based on said fitness function; and

(iii) refining said initial sub-set of M compounds based on said fitness function, thereby selecting said M compounds.

11. (Previously Presented) The method of claim 10, wherein step (g) comprises:

(i) selecting an initial sub-set of at least one K compound from said focused library of compounds;

(ii) evaluating said initial sub-set of at least one K compounds based on said fitness function; and

(iii) refining said initial sub-set of at least one K compound based on the fitness function, thereby selecting said at least one K compound.

12. (Previously Presented) The method of claim 11, wherein said fitness function is related to diversity of a collection of compounds, and wherein step (c)(ii) comprises evaluating a diversity of said initial sub-set of M compounds, and wherein step (c)(iii) comprises refining said initial sub-set of M compounds to increase said diversity of said M compounds

13. (Previously Presented) A computer implemented method of analyzing a non-enumerated virtual library, comprising:

(a) randomly selecting a set of N reagent combinations from the non-enumerated virtual library, wherein said selected N reagent combinations represent a set of N compounds;

(b) enumerating said set of N compounds;

(c) selecting M compounds from said set of N enumerated compounds wherein the selection of M compounds from said set of N enumerated compounds is based on at least one fitness function selected from similarity, diversity, and presence or absence at least one characteristic wherein selection comprises:

(i) selecting an initial sub-set of M compounds from said set of N enumerated compounds;

(ii) evaluating said initial sub-set of M compounds based on said fitness function which comprises evaluating a diversity of said initial sub-set of M compounds; and

(iii) refining said initial sub-set of M compounds based on said fitness function to increase said diversity of said M compounds, thereby selecting said M compounds;

(d) deconvoluting said M compounds into their associated building blocks;

(e) generating said focused library of at least one compound based on said building blocks; and

(f) enumerating at least one compound in said focused library of at least one compound;

(g) selecting at least one K compound from said focused library of compounds based on said fitness function by:

(i) selecting an initial sub-set of at least one K compound from said focused library of compounds;

(ii) evaluating said initial sub-set of at least one K compounds based on said fitness function thereby evaluating the diversity of said initial sub-set of K compounds ;

(iii) refining said initial sub-set of at least one K compound based on the fitness function to increase the diversity of said K compounds, thereby selecting said at least one K compound; and

(iv) outputting a list of said at least one K compound; and

(h) synthesizing said at least one K compound.

14. (Previously Presented) The method of claim 8, wherein step (c) comprises:

(i) characterizing said N enumerated compounds;

(ii) evaluating said characterized N enumerated compounds based on said fitness function;

(iii) ranking said characterized N enumerated compounds based on said evaluation; and

(iv) selecting said M compounds based on said ranking.

15. (Previously Presented) The method of claim 14, wherein said focused library of at least one compound comprises a plurality of compounds, wherein step (g) comprises:

(i) characterizing said compound of said focused library of compounds;

(ii) evaluating said characterized compound of said focused library of compounds based on said fitness function;

(iii) ranking said characterized compounds of said focused library of compounds based on said evaluation; and

(iv) selecting said K compounds based on said ranking.

16. (Previously Presented) The method of claim 15, wherein step (c)(i) comprises characterizing said N enumerated compounds using a set of molecular descriptors.

17. (Previously Presented) The method of claim 16, wherein step (g)(i) comprises characterizing compounds of said enumerated focused library of compounds using said set of molecular descriptors.

18. (Previously Presented) The method of claim 15, wherein said fitness function is related to a similarity to one or more query structures, and wherein step (c)(ii) comprises evaluating similarity between said N enumerated compounds and said one or more query structures.

19. (Previously Presented) The method of claim 18, wherein at least one of the following similarity measures is used in step (c)(ii) for evaluating similarity between each compounds and said one or more query structures:

(1) similarity in number of atoms, bonds and rings of the same types;

(2) similarity in shape and surface characteristics;

(3) similarity in electron density distribution;

(4) similarity based on common substructure;

(5) similarity based on the presence and orientation of pharmacophoric groups;

(6) similarity in binding affinity; and

(7) similarity in degree of conformational overlap with a know receptor binder.

20. (Previously Presented) A computer implemented method of analyzing a non-enumerated virtual library, comprising:

(a) randomly selecting a set of N reagent combinations from the non-enumerated virtual library, wherein said selected N reagent combinations represent a set of N compounds;

(b) enumerating said set of N compounds;

(c) selecting M compounds from said set of N enumerated compounds wherein the selection of M compounds from said set of N enumerated compounds is based on at least one fitness function selected from similarity, diversity, and presence or absence at least one characteristic whereby selection comprises:

(i) characterizing said N enumerated compounds;

(ii) evaluating said characterized N enumerated compounds based on said fitness function which is related to a similarity between said N enumerated compounds and said one or more query structures;

(iii) ranking said characterized N enumerated compounds based on said evaluation; and

(iv) selecting said M compounds based on said ranking.

(d) deconvoluting said M compounds into their associated building blocks;

(e) generating said focused library of at least one compound based on said building blocks; and

(f) enumerating at least one compound in said focused library of at least one compound;

(g) selecting at least one K compound from said focused library of compounds based on said fitness function by :

(i) characterizing said compound of said focused library of compounds;

(ii) evaluating said characterized compound of said focused library of compounds based on said fitness function thereby evaluating similarity between compounds of said enumerated focused library of compounds and said one or more query structures wherein the same similarity measure is used for evaluating similarity in step (c)(ii);

(iii) ranking said characterized compounds of said focused library of compounds based on said evaluation;

(iv) selecting said K compounds based on said ranking; and

(v) outputting a list of said at least one K compound; and

(h) synthesizing said at least one K compound.

21. (Previously Presented) The method of claim 14, wherein said fitness function is related to at least one desired characteristic, and wherein step (c)(ii) comprises evaluating N enumerated compounds to determine an extent to which the N enumerated compounds possess the at least one desired characteristic.

22. (Previously Presented) The method of claim 21, wherein the at least one desired characteristic comprises at least one of the following:

(1) a desired physical property;

(2) a desired chemical property;

(3) a desired functional property; and

(4) a desired bioactive property.

23. (Previously Presented) A computer based system for analyzing a non-enumerated virtual library, comprising:

means for randomly selecting a set of N reagent combinations from the virtual library, wherein said selected N reagent combinations represent a set of N compounds;

means for enumerating said set of N compounds;

means for selecting M compounds of said set of N enumerated compounds based on a fitness function;

means for deconvoluting said M compounds into their associated building blocks;

means for generating a said focused library of compounds based on said building blocks;

means for enumerating a plurality of said compounds of said focused library of compounds; and

means for selecting at least one K compound of said enumerated compounds of said focused library based on the fitness function,

wherein at least one selected K compound is synthesized.

24. (Previously Presented) A computer program product comprising a computer useable medium having computer program logic recorded thereon for enabling a processor to analyze a non-enumerated virtual library, the computer program logic comprising:

a first function that enables the processor to randomly select a set of N reagent combinations from the virtual library, wherein said selected N reagent combinations represent a set of N compounds;

a second function that enables the processor to enumerate said set of N compounds;

a first function that enables the processor to select M compounds of said set of N enumerated compounds based on a fitness function;

a third function that enables the processor to deconvolute said M compounds into their associated building blocks;

a fourth function that enables the processor to generate said focused library based on said building blocks;

a fifth function that enables the processor to enumerate a plurality of said compounds of said focused library; and

a sixth function that enables the processor to select at least one K compound of said enumerated compounds of said focused library based on the fitness function,

wherein at least one selected K compound is synthesized.

25. (Previously Presented) A computer implemented method of analyzing an enumerated virtual library, comprising:

(a) randomly selecting a set of N enumerated compounds from the enumerated virtual library;

(b) selecting M compounds from said set of N enumerated compounds wherein the selection of M compounds from said set of N enumerated compounds is based on at least one fitness function:

(c) deconvoluting said M compounds into associated building blocks;

(d) extracting said enumerated focused library based on said building blocks; said enumerated focused library including S enumerated compounds;

(e) selecting at least one K compound from said S enumerated compounds, wherein $K < S$; and

(f) synthesizing said at least one selected K compound.

26. (Previously Presented) The method of claim 25, wherein step (e) further comprises outputting a list of said at least one K compound.

31. (Previously Presented) The method of claim 25, wherein the at least one fitness function in step (b) is selected from similarity, diversity, and presence or absence at least one characteristic.

32. (Previously Presented) The method of claim 31, wherein step (e) further comprises selecting at least one K compound from said S enumerated compounds based on said fitness function.

34. (Previously Presented) The method of claim 32, wherein step (b) comprises:

(i) selecting an initial sub-set of M compounds from said set of N enumerated compounds;

(ii) evaluating said first sub-set of M enumerated compounds based on said fitness function; and

(iii) refining said initial sub-set of M enumerated compounds based on said fitness function, thereby selecting said M compounds.

35. (Previously Presented) The method of claim 34, wherein step (e) comprises:

(i) selecting an initial sub-set of at least one K compound from said S enumerated compounds;

(ii) evaluating said sub-set of at least one K compound based on said fitness function; and

(iii) refining said sub-set of at least one K compound based on said fitness function, thereby selecting said at least one K compound.

36. (Previously Presented) The method of claim 35, wherein said fitness function is related to a diversity of a collection of compounds, and wherein step (b)(ii) comprises evaluating a diversity of said sub-set of M enumerated compounds, and wherein step (b)(iii) comprises refining said sub-set of M enumerated compounds to increase the diversity of said sub set of M enumerated compounds.

37. (Previously Presented) The method of claim 36, wherein said initial sub-set of at least one K compound comprises a plurality of K compounds, wherein step (e)(ii) comprises evaluating the diversity of said initial sub-set of K compounds, and wherein step (e)(iii) comprises refining said initial sub-set of K compounds to increase the diversity of said K compounds.

38. (Previously Presented) The method of claim 32, wherein step (b) comprises:

(i) characterizing said set of N enumerated compounds;

(ii) evaluating said characterized set of N enumerated compounds based on said fitness function;

(iii) ranking said characterized set of N enumerated compounds; and

(iv) selecting said M compound of said set of N enumerated compounds based on said ranking.

39. (Previously Presented) The method of claim 38, wherein step (e) comprises:

(i) characterizing said S enumerated compounds;

(ii) evaluating said characterized S enumerated compounds based on said fitness function;

(iii) ranking said characterized S enumerated compounds; and

(iv) selecting said at least one K compound of said S enumerated compounds based on said ranking.

40. (Previously Presented) The method of claim 39, wherein step (b)(i) comprises characterizing said set of N enumerated compounds using a set of molecular descriptors.

41. (Previously Presented) The method of claim 40, wherein step (b)(i) comprises characterizing said S enumerated compounds using said set of molecular descriptors,

42. (Previously Presented) The method of claim 38, wherein said fitness function is related to a similarity to one or more query structures, and wherein step (b)(ii) comprises evaluating a similarity between compounds of said set of N enumerated compounds and the one or more query structures.

43. (Previously Presented) The method of claim 42, wherein at least one of the following similarity measures is used in step (b)(ii) for evaluating similarity between said set of N enumerated compounds and the one or more query structures:

(1) similarity in number of atoms, bonds and rings of the same types;

(2) similarity in shape and surface characteristics;

(3) similarity in electron density distribution;

(4) similarity based on common substructure;

(5) similarity based on the presence and orientation of pharmacophoric groups;

(6) similarity in binding affinity; and

(7) similarity in degree of conformational overlap with a know receptor binder.

44. (Previously Presented) The method of claim 42, wherein step (e)(ii) comprises evaluating similarity between said S enumerated compounds and the one or more query structures, and wherein the same similarity measure is used for evaluating similarity in step (b)(ii) and step (e)(ii).

45. (Previously Presented) The method of claim 38, wherein said fitness function is related to at least one desired characteristic, and wherein step (b)(ii) comprises evaluating said set of N enumerated compounds to determine an extent that said N enumerated compounds possesses the at least one desired characteristic.

46. (Previously Presented) The method of claim 45, wherein said at least one desired characteristic comprises at least one of the following:

(1) a desired physical property;

(2) a desired chemical property;

(3) a desired functional property; and

(4) a desired bioactive property.

47. (Previously Presented) A computer based system for analyzing an enumerated virtual library, comprising:

means for randomly selecting a set of N enumerated from the enumerated virtual library;

means for selecting M compounds of said set of N enumerated compounds based on the fitness function;

means for deconvoluting said M compounds into their associated building blocks;

means for extracting an enumerated focused library, based on said associated building blocks from the enumerated virtual library, wherein said enumerated focused library includes S enumerated compounds; and

means for selecting at least one K compound of said S enumerated compounds based on the fitness function,

wherein at least one selected K compound is synthesized.

48. (Previously Presented) A computer program product comprising a computer useable medium having computer program logic recorded thereon for enabling a processor to analyze an enumerated virtual library, the computer program logic comprising:

a first function that enables the processor to randomly select a set of N enumerated compounds from the enumerated virtual library;

a second function that enables the processor to select M compounds of said set of N enumerated compounds based on the fitness function;

a third function that enables the processor to deconvolute said M compounds into associated building blocks;

means for extracting an enumerated focused library, based on said associated building blocks from the enumerated virtual library, wherein said enumerated focused library includes S enumerated compounds; and

a fourth function that enables the processor to select at least one K compound of said S enumerated compounds based on the fitness function; and

a fifth function that enables the processor to select at least one K compound from said S enumerated compounds, wherein $K < S$, wherein at least one selected K compound is synthesized.

EVIDENCE APPENDIX

This appeal does not rely on any evidence submitted pursuant to 37 C.F.R. § 1.130, 1.131, or 1.132 that has been entered by the Examiner.

RELATED PROCEEDINGS APPENDIX

None.